

APPENDIX A

CHEMISTRY AND FATE

This appendix discusses the physical nature of specific chemicals used in dry and machine wetcleaning operations. Perchloroethylene (PCE) and hydrocarbon (HC) solvents are used at high concentrations in drycleaning. In machine wetcleaning, the detergents and soaps are chemical mixtures, typically containing numerous chemicals and water. Most of the formulations are trade secrets; therefore, the individual chemical concentrations are unknown. Nor is it known how representative the formulations considered in this report will be of the potential universe of formulations in existence. The following provides information on PCE, HC, and various chemicals that machine wetcleaning (MWC) formulations may contain. It is important to remember that the actual constituents of MWC formulations may vary significantly. First, this appendix describes the types of information that are provided for each chemical, including a glossary of chemical properties, or terms, presented in Exhibit A-1. These descriptions highlight chemical and physical properties, safety hazard factors, and environmental consequences. Following these descriptions, Exhibit A-2 lists the name, Chemical Abstracts Service (CAS) Registry Number, and common synonyms for each chemical. A Chemical Properties and Information Summary for each chemical lists its physical properties and safety hazard factors. Sections A.2, A.3, and A.4 summarize the environmental fate of PCE, HC, and machine wetcleaning chemicals, respectively.

A.1 CHEMICAL PROPERTIES AND INFORMATION

For each chemical identified, there is a corresponding summary of its chemical properties and relevant information. All information in these summaries was obtained by searching standard references, listed at the end of this chapter. These summaries contain information on the chemical and physical properties listed in Exhibit A-1.

The summaries of the chemicals' property values acquired from the standard references are designated as measured (M) (i.e., the data in these references were experimentally determined) or estimated (E). Terms and concepts such as synonyms and the role of the chemical in the cleaning process have no such designation since these are not values that can be measured.

Because information was proprietary, and therefore confidential, there were negligible or no data in the standard references for certain chemicals. Therefore, many of the values for the physical and chemical properties of these chemicals needed to be estimated. These estimations were obtained using several programs accessed through the Estimation Programs Interface (EPI), available from Syracuse Research Corporation (SRC, 1993a and 1993b). The EPI uses the structure of the chemical for input to eight chemical property estimation programs. The programs used to complete the individual Chemical Properties and Information summaries are as follows:

- Octanol-Water Partition Coefficient Program (LOGKOW) (Meylan and Howard, 1995).
- Henry's Law Constant Program (HENRY) (Meylan and Howard, 1991).
- Soil Sorption Coefficient Program (PCKOC) (Meylan et al., 1992).
- Melting Point, Boiling Point, Vapor Pressure Estimation Program (MPBPVP).

Exhibit A-1. Glossary of Chemical and Physical Properties

Term	Definition
Chemical Abstracts Service Registry Number (CAS#)	A unique identification code, up to ten digits long, assigned to each chemical registered by the Chemical Abstracts Service. The CAS# is useful when searching for information on a chemical with more than one name.
Synonyms	Alternative names commonly used for the chemical.
Molecular Weight	A summation of the individual atomic weights based on the numbers and kinds of atoms present in a molecule of a chemical substance. For polymers, this may include molecular weight distributions, ranges, and averages. Typical unit is grams per mole (g/mol).
Melting Point	The temperature at which a substance changes from the solid to the liquid state. Typical unit is °C.
Vapor Pressure	The pressure exerted by a chemical in the vapor phase in equilibrium with its solid or liquid forms. It provides an indication of the relative tendency of a substance to volatilize. Typical unit is mm Hg.
Octanol-Water Partition Coefficient ($\text{Log}_{10} K_{ow}$)	Provides a measure of the extent to which a chemical partitions between water and octanol (as a surrogate for lipids) at equilibrium. It is an important parameter because it provides an indication of a chemical's water solubility and its propensity to partition in aquatic organisms or sorb to soil and sediment. The higher the $\text{Log } K_{ow}$, the more likely a chemical is to move from water to lipids.
Bioconcentration Factor (BCF)	Provides a measure of the extent of chemical partitioning at equilibrium between a biological medium such as fish tissue or plant tissue and an external medium such as water. The higher the BCF, the greater the accumulation in living tissue is likely to be.
Henry's Law Constant	Provides a measure of the extent of chemical partitioning between air and water at equilibrium; estimated by dividing the vapor pressure of a sparingly water soluble chemical substance by its water solubility. The higher the Henry's Law constant, the more likely a chemical is to volatilize than to remain in water.
Applicable Function	The primary function(s) of the chemical in the cleaning operation.
Molecular Formula and Physical Structure of the Chemical	A description of the number and type of each atom in the chemical, how the atoms are arranged, and the types of bonds between atoms.
Boiling Point	The temperature at which a liquid under standard atmospheric pressure (or other specified pressure) changes from a liquid to a gaseous state. It is an indication of the volatility of a substance. The distillation range in a separation process, the temperature at which the more volatile liquid of a mixture forms a vapor, is used for mixtures in the absence of a boiling point. Typical unit is °C.
Density	The mass of a liquid, solid, or gas per unit volume of that substance, i.e., the mass in grams contained in 1 cubic centimeter of a substance at 20°C and 1 atmosphere. Typical unit is g/cm ³ .
Flash Point	The minimum temperature at which a liquid gives off sufficient vapor to form an ignitable mixture with air near the surface of the liquid or within the test vessel used.
Safety Hazard Factors	Discussed in detail below.

- Water Solubility Estimation Program (WSKOW) (Meylan et al., 1996).
- Sewage Treatment Plant Model (STP), a fugacity model for estimating the efficiency of pollutant removal (Clark et al., 1995).

The accuracy of these programs is not established in all cases, but the listed programs are considered the best methods currently available. The reference section at the end of this appendix lists journal articles discussing the development and use of these programs (except the MPBPVP program). A user's guide also is available for the EPI and each program. Any property values determined using these programs are designated as estimated (E). It should be noted that the water solubility estimation program has an anticipated margin of error of plus or minus one order of magnitude. The Log K_{ow} is expected to be accurate to 0.1 log units for most compounds, although the PCK_{oc} is likely to be somewhat less accurate due to the complex nature of the soil/sediment sorption phenomena.

For several chemicals, data were not available in any of the primary sources, and EPI estimation methods were not performed because the complex nature of the chemical (e.g., chemicals with ranges of carbon atoms) skewed the estimation results. For these chemicals, chemical and physical data had to be estimated based on structure-activity relationships (i.e., comparison with analogous chemicals with known properties). In addition, some properties were estimated from best chemical judgment based on the class of compounds to which the specific chemical belongs. Any property values determined by this comparison method are designated by an E. Any chemical and physical property values that still could not be estimated have been designated as not available.

Exhibit A-2 contains the dry and machine wetcleaning chemicals under consideration with their common synonyms and specified CAS Registry Number (CAS, 1993). Immediately following the exhibit are individual Chemical Properties and Information summaries for each chemical.

Exhibit A-2. Chemicals Utilized in Dry and Machine Wetcleaning Operations

Chemical Name	CAS No.	Chemical Synonyms
Acetic acid (WC)	64-19-7	Acetic acid glacial; vinegar; ethanoic acid
Cellulose gum (WC)	9004-32-4	Sodium carboxymethylcellulose; CMC; carboxymethylcellulose, sodium salt; CM cellulose
Citric acid (WC)	77-92-9	1,2,3-Propane tricarboxylic acid; 2-hydroxy-hydroxytricarballic acid
Cocamidopropyl betaine (WC)	61789-40-0	1-Propanaminium, 3-amino-N-(carboxymethyl)-N, N-dimethyl-, N-coco acyl derivatives, inner salts; cocamidopropyl dimethyl glycine
Ethoxylated sorbitan monodecanoate (WC)	9005-64-5	Polyoxyethylene (20) sorbitan monolaurate; sorbitan, monodecanoate, poly(oxy-1, 2-ethanediyl) derivatives
Lauric acid diethanolamide (WC)	120-40-1	Lauramide DEA; N,N-bis (2-hydroxyethyl) lauramide
Methyl 2-sulfolaurate, sodium salt (WC)	4337-75-1	Sodium methyl 2-sulfolaurate; N-lauroyl-N-methyl-aurine, sodium salt; ethanesulfonic acid, 2-[methyl (1-oxododecyl) amino]-, sodium salt
Perchloroethylene (DC)	127-18-4	Tetrachloroethylene; perchlor; perc; carbon bichloride; carbon dichloride; ethylene tetrachloride; tetrachloroethene
Sodium carbonate (WC)	497-19-8	Carbonic acid; sodium salt; soda ash; Solvay soda
Sodium citrate (WC)	68-04-2	Trisodium citrate; 1,2,3-propane tricarboxylic acid; 2-hydroxy-trisodium salt
Sodium laureth sulfate (WC)	9004-82-4	Ethoxylated sodium laureth sulfate; ethoxylated sodium lauryl ethyl sulfate; poly(oxy-1, 2-ethanediyl)-sulfo-(dodecyloxy)-, sodium salt
Sodium lauryl isethionate (WC)	7381-01-3	Sodium ethyl 2-sulfolaurate; sodium dodecoylisethionate; dodecanoic acid, 2-sulfoethylester, sodium salt
Stoddard solvent (Petroleum) (DC)	8052-41-3	Solvent naphtha; white spirits; mineral spirits
140°F solvent (Petroleum) (DC)	64742-88-7	Solvent naphtha (petroleum), medium aliphatic
DF-2000 solvent (DC)		Hydrotreated heavy naphtha (petroleum); naphtha (petroleum), hydrotreated and heavy, nonaromatic

Acetic Acid
CAS# 64-19-7

Chemical Properties and Information	
<p><i>Synonyms:</i> Acetic acid glacial, vinegar, ethanoic acid</p>	
$\text{CH}_3\overset{\text{O}}{\parallel}\text{COH}$	
<p><i>Molecular Weight:</i> 60.05 <i>Melting Point:</i> 16.7°C (M) <i>Boiling Point:</i> 118°C (M) <i>Flash Point:</i> 103°F (closed cup) (M)</p>	<p><i>Molecular Formula:</i> C₂H₄O₂</p>
<p><i>Vapor Pressure:</i> 10mg Hg (at 17.1°C) (M)</p>	<p><i>Physical State:</i> Liquid</p>
<p><i>Water Solubility:</i> Miscible in water in all proportions (M)</p>	<p><i>Density:</i> 1.049 g/L (at 25°C) (M)</p>
<p><i>Other Solubilities:</i> Miscible with alcohol, glycerol, ether, carbon tetrachloride</p>	<p><i>Log₁₀K_{OW}:</i> - 0.09 <i>Log₁₀BCF:</i> <1</p>
<p><i>Applicable Function:</i> pH adjuster</p>	

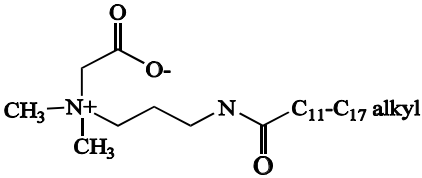
Cellulose Gum
CAS# 9004-32-4

Chemical Properties and Information	
<p><i>Synonyms:</i> sodium carboxymethylcellulose; CMC; carboxymethylcellulose, sodium salt; CM cellulose</p>	
$\text{R-O-CH}_2\text{COONa}$ <p>R=(C₆H₁₀O₅)</p>	
<p><i>Molecular Weight:</i> High (>10,000)</p>	<p><i>Molecular Formula:</i> varies</p>
<p><i>Melting Point:</i> not available</p>	<p><i>Physical State:</i> Solid</p>
<p><i>Boiling Point:</i> not available</p>	<p><i>Density:</i> 0.75 g/cm³</p>
<p><i>Flash Point:</i> Not available</p>	<p><i>Log₁₀K_{OW}:</i> n/a</p>
<p><i>Vapor Pressure:</i> <10⁻⁶ mm Hg (E)</p>	<p><i>Log₁₀BCF:</i> n/a</p>
<p><i>Water Solubility:</i> Soluble (M)</p>	<p><i>Other Solubilities:</i> Insoluble in organic liquids</p>
<p><i>Applicable Function:</i> soil suspender</p>	

Citric Acid
CAS# 77-92-9

Chemical Properties and Information	
<i>Synonyms:</i> 1, 2, 3-Propane tricarboxylic acid, 2-hydroxy-hydroxytricarballic acid	$\text{HOC}(\text{CH}_2\text{COOH})_2\text{COOH}$ <i>Molecular Formula:</i> $\text{C}_6\text{H}_8\text{O}_7$
<i>Molecular Weight:</i> 191.12	<i>Physical State:</i> solid
<i>Melting Point:</i> 153°C (loses water) (M)	<i>Density:</i> 1.542 g/cm ³
<i>Boiling Point:</i> Decomposes (M)	<i>Log₁₀K_{OW}:</i> -1.67
<i>Flash Point:</i> Not available	<i>Log₁₀BCF:</i> <1
<i>Vapor Pressure:</i> <10 ⁻⁶ mm Hg	<i>Water Solubility:</i> 592 g/L @20°C (M)
<i>Applicable Function:</i> pH control	<i>Other Solubilities:</i> Soluble in alcohol and ether.

Cocamidopropyl betaine
CAS# 61789-40-0

Chemical Properties and Information	
<i>Synonyms:</i> 1-Propanaminium, 3-amino-N-(carboxymethyl)-N,N-dimethyl-, N-coco acyl derivatives, inner salts; cocamidopropyl dimethyl glycine	
<i>Molecular Weight:</i> 342.53	<i>Molecular Formula:</i> $\text{C}_{19}\text{H}_{38}\text{N}_2\text{O}_3$ (for C-11)
<i>Vapor Pressure:</i> Negligible (E)	<i>Physical State:</i> Solid (E)
<i>Water Solubility:</i> > 200 g/L at 25°C (E) (dispersible)	<i>Log₁₀K_{OW}:</i> -4.9
<i>Other Solubilities:</i> Slightly soluble in some organic solvents	<i>Log₁₀BCF:</i> <1
<i>Applicable Function:</i> amphoteric surfactants	

Ethoxylated Sorbitan Monodecanoate

CAS# 9004-64-5

Chemical Properties and Information	
<i>Synonyms:</i> Polyoxyethylene (20) sorbitan monolaurate; sorbitan, monodecanoate, poly(oxy-1, 2-ethanediyl) derivatives	<i>Molecular Formula:</i> C ₅ H ₁₁₄ O ₂₆ <i>Molecular Weight:</i> 1180 <i>Physical State:</i> Liquid <i>Density:</i> 1.1g/cm ³
<i>Melting Point:</i> Not available	<i>Log₁₀K_{OW}:</i> n/a
<i>Boiling Point:</i> Not available	<i>Log₁₀BCF:</i> n/a
<i>Flash Point:</i> 148°C (closed cup) (M)	<i>Vapor Pressure:</i> <10 ⁻⁶ mm HG
<i>Water Solubility:</i> completely soluble (M); 1000 g/L (E)	<i>Applicable Function:</i> non-ionic surfactant
<i>Other Solubilities:</i> Soluble in alcohol, ethyl acetate, and dioxane. Insoluble in mineral oil and mineral spirits.	

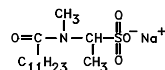
Lauric Acid Diethanolamide

CAS# 120-40-1

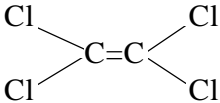
Chemical Properties and Information	
<i>Synonyms:</i> Lauramide DEA; N, N-bis (2-hydroxyethyl) lauramide; N, N-bis (2-hydroxyethyl) Dodecanamide	<i>Molecular Formula:</i> C ₁₆ H ₃₃ NO ₃ <i>Structural Formula:</i> CH ₃ (CH ₂) ₁₀ CON(CH ₂ CH ₂ OH) ₂
<i>Molecular Weight:</i> 287.17	<i>Physical State:</i> Solid
<i>Melting Point:</i> 50°C (E)	<i>Density:</i> 0.979 g/cm ³
<i>Boiling Point:</i> 359°C (M)	<i>Log₁₀K_{OW}:</i> n/a
<i>Flash Point:</i> Not Available	<i>Log₁₀BCF:</i> n/a
<i>Vapor Pressure:</i> <10 ⁻⁶ mm Hg (E)	<i>Water Solubility:</i> 0.69 g/L (M)
<i>Other Solubilities:</i> Soluble in polar organic solvents	<i>Applicable Function:</i> surfactant

Methyl 2-Sulfolaurate, Sodium Salt
CAS# 4337-75-1

Chemical Properties and Information	
<p><i>Synonyms:</i> sodium methyl 2-sulfolaurate; N-lauroyl-N-methyl-taurine, sodium salt; ethanesulfonic acid, 2-[methyl (1-oxododecyl) amino]-, sodium salt</p>	
<p><i>Molecular Weight:</i> 343.2</p>	<p><i>Molecular Formula:</i> $C_{15}H_{30}NO_4S_2Na$</p>
<p><i>Melting Point:</i> 207 - 208°C</p>	<p><i>Physical State:</i> solid</p>
<p><i>Boiling Point:</i> Decomposes (E)</p>	<p><i>Density:</i> >1g/cm³</p>
<p><i>Flash Point:</i> n/a</p>	<p><i>Log₁₀K_{OW}:</i> n/a</p>
<p><i>Vapor Pressure:</i> <10⁻⁶ mm Hg (E)</p>	<p><i>Log₁₀BCF:</i> n/a</p>
<p><i>Other Solubilities:</i> Soluble in polar organic solvents</p>	<p><i>Water Solubility:</i> Dispersible (E)</p>
<p><i>Applicable Function:</i> dispersant</p>	



Perchloroethylene
CAS# 127-18-4

Chemical Properties and Information	
<p><i>Synonyms:</i> tetrachloroethylene, perchlor, perc, carbon bichloride, carbon dichloride, ethylene tetrachloride, tetrachloroethene</p>	<p><i>Molecular Formula:</i> C₂Cl₄</p> <div style="text-align: center;">  </div>
<p><i>Molecular Weight:</i> 165.82</p>	<p><i>Physical State:</i> Liquid</p>
<p><i>Boiling Point:</i> 121.07°C</p>	<p><i>Log₁₀K_{OW}:</i> 3.40</p>
<p><i>Vapor Pressure:</i> 18.5 mm Hg@25°C</p>	<p><i>BCF:</i> 49/40 (M)</p>
<p><i>Other Solubilities:</i> Soluble in most organic solvents; dissolves a wide range of organic compounds including organic acids, fats, oils, rubber, tars, and resins; solubilizes a number of inorganic materials including sulfur, iodine, mercuric chloride, and aluminum chloride</p>	<p><i>Henry's Law Constant:</i> 0.0184 atm/m³-mole</p>
<p><i>Freezing Point:</i> -22.35°C</p>	<p><i>Water Solubility:</i> 150 mg/Kg</p>
<p><i>Flashpoint:</i> Not flammable</p>	<p><i>Hildebrand Solubility</i> is 9.3 cal^{1/2}/cm^{3/2}</p>
<p><i>Specific Gravity:</i> 1.6@25°C</p>	<p><i>Surface Tension:</i> 31.3 dynes/cm²</p>
<p><i>Refractive Index:</i> 1.503</p>	<p><i>Dielectric Constant:</i> 2.280</p>
<p><i>Viscosity:</i> 0.798 cP@30°C</p>	<p><i>Vapor Density:</i> 5.8 (air=1)</p>
<p><i>Evaporation Rate:</i> 2.10 (butyl acetate=1)</p>	<p><i>Heat of Vaporization:</i> 9.47 cal/g@25°C</p>
<p><i>Odor Threshold:</i> 50 ppm</p>	<p><i>Specific Heat:</i> 35.01 cal/°K-mole</p>
<p><i>Applicable Function:</i> solvent</p>	<p><i>Kauri Butanol Number:</i> 90</p>

Sodium Carbonate

CAS# 497-19-8

Chemical Properties and Information	
<i>Synonyms:</i> carbonic acid, sodium salt, soda ash, Solvay soda	<i>Molecular Formula:</i> NaCO ₃
<i>Molecular Weight:</i> 83	<i>Physical State:</i> Solid
<i>Melting Point:</i> 851 °C (M)	<i>Density:</i> 2.53 g/cm ³ (M)
<i>Boiling Point:</i> Decomposes (M)	<i>Log₁₀K_{OW}:</i> 0.0
<i>Flash Point:</i> Not Available	<i>Log₁₀BCF:</i> <1
<i>Vapor Pressure:</i> <10 ⁻⁶ mm Hg (E)	<i>Water Solubility:</i> 71 g/L (M)
<i>Other Solubilities:</i> Soluble in glycerol; insoluble in alcohol and acetone	<i>Applicable Function:</i> solubilizer, detergent aid

Sodium Citrate

CAS# 68-04-2

Chemical Properties and Information	
<i>Synonyms:</i> Trisodium citrate; 1, 2, 3-propane tricarboxylic acid, 2-hydroxy-trisodium salt	$ \begin{array}{c} \text{O} \quad \quad \text{OH} \quad \quad \text{O} \\ \parallel \quad \quad \quad \quad \parallel \\ \text{NaOOCCH}_2\text{CCH}_2\text{CONa} \\ \\ \text{O}=\text{CONa} \end{array} $
<i>Molecular Weight:</i> 258.07	<i>Molecular Formula:</i> C ₆ H ₅ NaO ₇
<i>Melting Point:</i> Becomes anhydrous at 150 °C (M)	<i>Physical State:</i> solid
<i>Boiling Point:</i> Not Applicable	<i>Density:</i> Not Available
<i>Flash Point:</i> Not Available	<i>Log₁₀K_{OW}:</i> - 1.67
<i>Vapor Pressure:</i> Not Available	<i>Log₁₀BCF:</i> <1
<i>Water Solubility:</i> 760 g/L (M)	<i>Other Solubilities:</i> Insoluble in alcohol
<i>Applicable Function:</i> emulsifier aid	

Sodium Laureth Sulfate

CAS# 9004-82-4

Chemical Properties and Information	
<i>Synonyms:</i> Ethoxylated sodium laureth sulfate; ethoxylated sodium lauryl ethyl sulfate; poly(oxy-1, 2-ethanediyl)-sulfo-(dodecyloxy)-, sodium salt	<i>Molecular Formula:</i> $(C_2H_4O)_n C_{12}H_{25}O_4S_7Na$ <i>Molecular Weight:</i> varies with degree of ethoxylation (>330) <i>Physical State:</i> solid
<i>Melting Point:</i> not available	<i>Density:</i> >1 g/cm ³
<i>Boiling Point:</i> not available	<i>Log₁₀K_{OW}:</i> n/a
<i>Flash Point:</i> not available	<i>Log₁₀BCF:</i> n/a
<i>Water Solubility:</i> dispersible (E)	<i>Vapor Pressure:</i> <10 ⁻⁶ mm Hg (E)
<i>Other Solubilities:</i> Soluble in polar organic solvents and alcohols	<i>Applicable Function:</i> surfactant

Sodium Lauryl Isethionate

CAS# 7381-01-3

Chemical Properties and Information	
<i>Synonyms:</i> sodium ethyl 2-sulfolaurate; sodiumdodecyl-isethionate; dodecanoic acid, 2-sulfoethylester, sodium salt	$ \begin{array}{c} \text{O} \\ \parallel \\ \text{C}_{10}\text{H}_{21}\text{CHCO}^- \text{Na}^+ \\ \\ \text{O} \\ \\ \text{O}=\text{S} \begin{array}{c} \diagup \diagdown \\ \text{CH}_2\text{CH}_3 \end{array} \\ \parallel \\ \text{O} \end{array} $
<i>Molecular Weight:</i> 330.3	<i>Molecular Formula:</i> C ₁₄ H ₂₇ O ₅ S ₂ Na
<i>Melting Point:</i> 216 - 218 °C	<i>Physical State:</i> solid
<i>Boiling Point:</i> decomposes (E)	<i>Density:</i> >1 g/cm ³
<i>Flash Point:</i> not available	<i>Log₁₀K_{OW}:</i> n/a
<i>Vapor Pressure:</i> <10 ⁻⁶ mm Hg (E)	<i>Log₁₀BCF:</i> n/a
<i>Water Solubility:</i> Dispersible (E)	<i>Other Solubilities:</i> soluble in polar organics
<i>Applicable Function:</i> surfactant	

Stoddard Solvent
CAS# 8052-41-3

Chemical Properties and Information	
<i>Synonyms:</i> Solvent naphtha; white spirits; that mineral spirits	<i>Definition:</i> A colorless, refined petroleum distillate is free from rancid or objectionable odors and that boils in the range of approx. 149 - 205 °C.
<i>Molecular Weight:</i> 126.24 (LOWWT, C ₉ H ₁₈)	<i>Molecular Formula:</i> C _n 2 _{n+2} (paraffins) and C _n H _{2n} (cycloparaffins) (typical)
<i>Boiling Point:</i> 150-210 °C; 149-208 °C (Merck) <i>Freezing Point:</i> -70 °C	<i>Log₁₀K_{ow}:</i> 4.76*
<i>Vapor Pressure:</i> 2 mm Hg at 20 °C	<i>Water Solubility:</i> 0.0024 g/L*
<i>Vapor Density:</i> 4.9 (air = 1)	<i>Specific Gravity:</i> 0.75 - 0.85
<i>Surface Tension:</i> 0.027 - 0.05 N/m	<i>Refractive Index:</i> 1.4278
<i>Flash Point:</i> 41 °C; 38 °C (Merck)	<i>Evaporation Rate:</i> 0.12 (butyl acetate = 1)
<i>Heat of Vaporization:</i> 284.3 J/g <i>Upper Explosive Limit:</i> 6.0% (Chemcentral) <i>Lower Explosive Limit:</i> 1.0%	<i>Reactivity:</i> 0 <i>Flammability:</i> 2 <i>Ignitability:</i> Y; Autoignition temp: 232 °C
<i>Kauri Butanol Number:</i> 27 - 45 <i>Dielectric Constant:</i> 2.00 - 3.00	<i>Applicable Function:</i> Cleaning solvent

*Water solubility and log K_{ow} were estimated using the EPI program (SRC) for nonane (C₉H₂₀) representing the most soluble component of Stoddard solvent. The water solubility average estimate for 23 C₉ paraffins and cycloparaffins is 2.5 - 4.7x10⁻⁵ g/kg.

140°F Solvent
CAS# 64742-88-7

Chemical Properties and Information	
<i>Synonyms:</i> Solvent naphtha (petroleum), medium aliphatic predominantly range <i>Molecular Weight:</i> 126.24 (LOWWT, C ₉ H ₁₈) <i>Boiling Point:</i> 183 - 199 °C Ashland 140) 191 - 203 °C (Chemcentral 140) 187-206 °C (Shell Sol 140) <i>Vapor Pressure:</i> 0.5 mm Hg at 20 °C (Chemcentral 140) <i>Vapor Density:</i> 5.4 (air = 1) (Ashland 140) <i>Flash Point:</i> 60 - 62.2 °C (typical) <i>Hildebrand Solubility Parameter:</i> 7.6 cal ^{1/2} /cm ^{3/2} (Chemcentral 140) <i>Kauri Butanol Number:</i> 30 - 31 <i>Dielectric Constant:</i> 2.04 (Shell Sol 140)	<i>Definition:</i> Saturated hydrocarbons obtained from the distillation of crude oil or natural gasoline having carbon numbers in the range of C9-C12 and boiling in the of 140 - 220 °C. <i>Molecular Formula:</i> C _n 2 _{n+2} (paraffins) and C _n H _{2n} (cycloparaffins) (typical) <i>Log₁₀K_{ow}:</i> 4.76* <i>Water Solubility:</i> 0.0024 g/L* <i>Specific Gravity:</i> 0.78 at 25 °C (typical) <i>Refractive Index:</i> 1.43 (Chemcentral 140) <i>Evaporation Rate:</i> 0.08<X<0.1 (typical, butyl acetate = 1) <i>Reactivity:</i> 0 <i>Flammability:</i> 2 <i>Ignitability:</i> Y <i>Applicable Function:</i> Lower flash point alternative to drycleaning chemicals

*Water solubility and log K_{ow} were estimated using the EPI program (SRC) for nonane (C₉H₂₀) representing the most soluble component of 140°F solvent. The water solubility average estimate for 23 C₉ paraffins and cycloparaffins is 2.5 - 4.7x10⁻⁵ g/Kg.

DF-2000 Solvent

Chemical Properties and Information	
<i>Synonyms:</i> Hydrotreated heavy naphtha (petroleum); Naphtha (petroleum), hydrotreated and heavy, nonarom.	<i>Definition:</i> A complex combination of hydrocarbons obtained by treating a petroleum fraction with hydrogen and catalyst. It consists of hydrocarbons having carbon numbers predominantly in the range of C6-C13 and boiling in the range of approx. 65-230 °C.
<i>Molecular Weight:</i> 84.16 (LOWWT, C ₆ H ₁₂)	<i>Molecular Formula:</i> C _n 2 _{n+2} (paraffins) and C _n H _{2n} (cycloparaffins) (typical)
<i>Boiling Point:</i> 191 - 205 °C (Exxon Chemical)	<i>Log₁₀K_{ow}:</i> 3.9*
<i>Freezing/Melting Point:</i> <-60 °C	<i>Water Solubility:</i> <0.01 at 15 °C
<i>Vapor Pressure:</i> 1 at 20 °C (E)	<i>Specific Gravity:</i> 0.77 at 15 °C
<i>Vapor Density:</i> 5.90 (Air = 1) (calculated)	<i>Refractive Index:</i> n/a
<i>Flash Point:</i> 64 °C (TCC) (typical)	<i>Evaporation Rate:</i> <0.1 (n-butyl acetate = 1)
<i>Viscosity:</i> 2.1 cSt at 15 °C (E)	<i>Reactivity:</i> 0
°C)(E)	<i>Flammability:</i> 2 (LEL: 1.3; UEL 8.8 @ 25
	<i>Ignitability:</i> Y; Autoignition temp: 338 °C (E)
	<i>Applicable Function:</i> Cleaning solvent

*Log K_{ow} was estimated using the EPI program (SRC) for hexane (C₆H₁₂) representing the most soluble component of DF-2000 Solvent.

A.2 PERCHLOROETHYLENE ENVIRONMENTAL FATE SUMMARY

PCE is expected to biodegrade slowly in water and in soils. Aerobic and anaerobic biodegradation, in water and soil, respectively, are estimated as taking months and hydrolysis as taking years. Actual biodegradation rates will depend upon local soil conditions. In one study, trichloroethylene, cis-1,2-dichloroethene, trans-1,2-dichloroethene, chloroethene, and dichloromethane were produced as PCE biodegraded over a 21-day period.

Groundwater contaminated by PCE has been found in a number of places; the contamination may take place because PCE is more dense and less viscous than water. PCE's migration potential from a landfill to groundwater is estimated as negligible to moderate and depends on local conditions. PCE is a classic groundwater contaminant.

PCE's rate of volatilization depends upon the depth and turbulence of surface water. Using a model that assumes a standard 1-meter depth stream, the volatilization potential is estimated as moderate. Sorption to soil and sediment is low. The estimated half-life of PCE in stream or river water is 1.4 hours. The estimated wastewater treatment removal efficiency, which depends mainly on volatilization, is 88 percent. Hydrolysis of PCE is expected to be slow compared with volatilization from surface water (Versar, 1987). In the presence of sunlight, PCE is also expected to photooxidize in water (Versar, 1987).

A.3 HYDROCARBON SOLVENT ENVIRONMENTAL FATE SUMMARY

Stoddard solvent is expected to biodegrade slowly, with aerobic and anaerobic biodegradation taking weeks to months. Migration to groundwater is negligible, and sorption to soil and sediment is very strong. The estimated half-life for volatilization from water in rivers is 1.58 hours; the half-life for volatilization from water in lakes is 6.11 days. The estimated removal efficiency in wastewater treatment is 95 percent. The estimated half-life resulting from atmospheric oxidation is five hours.

Stoddard solvent's stratospheric ozone depletion potential is zero (USEPA, 1992). However, Stoddard solvent is a potential VOC (lower level ozone) contributor and has global warming potential (USEPA, 1992).

The 140°F solvent is expected to biodegrade rapidly, with aerobic and anaerobic biodegradation taking days to weeks. Migration to groundwater is negligible, and sorption to soil and sediment is strong. The estimated half-life for volatilization from water in rivers is 1.3 hours; the half-life for volatilization from water in lakes is 5.2 days. The estimated removal efficiency in wastewater treatment is 99.9 percent due to high volatilization and biodegradation. The estimated half-life resulting from atmospheric oxidation is 9.4 hours.

The stratospheric ozone depletion potential of 140°F solvent is zero (USEPA, 1992). It is also a potential VOC (lower level ozone) contributor and has global warming potential (USEPA, 1992).

A.4 MACHINE WETCLEANING ENVIRONMENTAL FATE SUMMARY

Partial removal of chemicals from water often occurs during treatment in publicly owned treatment works (POTWs). Two frequently encountered removal mechanisms are adsorption to sludge and hydrolysis. Others include biodegradation and volatilization. An environmental fate summary (see Exhibit A-3) presents information on adsorption to soils and sediments, ultimate biodegradation, and percent removal in wastewater treatment and removal process.

Adsorption to soil and sediment is the tendency of a chemical to bind to the material at the bottom layer of a water body (e.g., a river bed). This is significant because chemicals trapped at the bottom of a river bed generally do not contaminate the drinking water supply.

Ultimate biodegradation, which occurs in water and soils, is the conversion of the carbon in an organic chemical to carbon dioxide. This occurs when microorganisms break down a chemical to its elemental state (e.g., carbon dioxide and ammonia). Once the chemical is in its elemental state, it is no longer of concern.

Exhibit A-3. Environmental Fate Information for Machine Wetcleaning Chemicals^a

Chemical Name	CAS Number	Adsorption to Soil and Sediment	Time for Biodegradation	% Removal in Wastewater Treatment
Acetic acid	64-19-7	low	days	90
Cellulose gum	9004-32-4	strong	weeks to months	50
Citric acid	77-92-9	low	days	90
Ethoxylated sorbitan monodecanoate	9005-64-5	moderate	days to weeks	90
Lauric acid diethanolamide	120-40-1	low	days to weeks	90
Methyl 2-sulfolaurate, sodium salt	4337-75-1	moderate	days to weeks	90
Sodium carbonate	497-19-8	unspecified	unspecified	zero
Sodium citrate	68-04-2	low	days	90
Sodium laureth sulfate	9004-82-4	unspecified	days to weeks	90
Sodium lauryl isethionate	7381-01-3	moderate	days to weeks	90

^a No information is available for cocoamidopropyl betaine.

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